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BSC

Scientific Analysis Administrative Change Notice

Complete only applicable items.

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4. Title:	Evaluation of Potential Impacts of Microbial Activity on Drift Chemistry				
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6. Approvals:

	Print Name and Sign	Date
Preparer:	G.H. Nieder-Westermann SIGNATURE ON FILE	06/06/05
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7. Affected Pages	8. Description of Change:
4-2	Added information Table 4.1-1 "Direct Inputs from Project Sources", add a last row to read: Parameter(s) or Information — Value(s) — Source ***Maximum surface dose rate due to gamma radiation*** — ***1160 rad/hour*** — ***BSC 2005 [DIRS 173426, Table 2*** This error was identified and corrected in ANL-EBS-MD-000038, Rev 01, ACN 01
4-2	Citation update Table 4.1-2 "Numeric Data from Outside Sources Used as Direct Inputs", 3rd column, 4th cell, change: *NIST 2003 [DIRS 171201]* To ***NIST 2004 [DIRS 171201]*** This error was identified in CR 5720
6-40	Citation update Table 6.5-2 "Complexation of AM^{3+} with Intermediate Metabolites", Footnote, change: *Source: NIST 2003 [DIRS 171201]* To ***Source: NIST 2004 [DIRS 171201]*** This error was identified in CR 5720

Table 4.1-1. Direct Inputs from Project Sources (Continued)

Parameter(s) or Information	Value(s)	Source
Under oxidizing conditions, Pu will be dominated by Pu(V) and Pu(VI) instead of Pu(IV)	–	BSC 2004 [DIRS 169425], Figure 6.5-5
Brine solutions ionic strength	10M	BSC 2004 [DIRS 169860], Section 6.1.3
Maximum surface dose rate due to gamma radiation	1,160 rad/hour	BSC 2005 [DIRS 173426], Table 2

4.1.2 Direct Inputs from Outside Sources

Table 4.1-2 lists the direct inputs (from outside sources) that were obtained from investigation activities such as measurement, testing, and analysis. Of these outside sources, the National Institute of Standards and Technology (NIST) maintains the database of reaction constants that is accepted by the scientific and engineering communities as established fact, and therefore the constants do not need to be qualified in accordance with YMP procedures. Data from the other two external sources listed in Table 4.1-2 and Table 4.1-3 are not established fact and are therefore demonstrated to be qualified for their intended use in Table 4.1-4 in accordance with Section 5.2.1.1 of AP-SIII.9Q.

Table 4.1-2. Numeric Data from Outside Sources Used as Direct Inputs

Parameter(s) or Information	Value(s)	Source
Upper temperature limit for microbial growth	110°C	Pedersen and Karlsson 1995 [DIRS 100810]
Concentration of O_2 for aquatic sediments above which anaerobic microbial reactions are completely inhibited	1 to 30 μM (approximately 0.4 to 10% atmospheric oxygen)	Wang and Van Cappellen 1996 [DIRS 171057], Table 3
Water activity levels at which bacteria can grow	0.75 to 1.00	Pedersen & Karlsson 1995 [DIRS 100810]
Complexation constants	See Table 6.5-2	NIST 2004 [DIRS 171201]
Growth of Yucca Mountain bacteria	See Table 6.3-1	Horn et al. 2004 [DIRS 171058]

Table 4.1-3. Information from Outside Sources, Other Than Data, Used as Direct Inputs

Information	Source
Water is essential for microbial growth.	Horn et al. 2004 [DIRS 171058]
There is negligible long-distance biocolloid transport in porous geologic media that are not significantly fractured.	DeFlaun et al. 1997 [DIRS 171060]
Table 6.1-1 – Nutritional Requirements of Microorganisms	Pedersen and Karlsson 1995 [DIRS 100810]

Now use $[RC]=K[R][C]$ and substitute in the above to obtain:

$$Fraction = \frac{K[R][C]}{[R]+K[R][C]} = \frac{K[C]}{1+K[C]}$$

This is equivalent to:

$$Fraction = 1-\frac{1}{1+K[C]} = \frac{1+K[C]-1}{1+K[C]} = \frac{K[C]}{1+K[C]} \qquad \text{(Eq. 6-5)}$$

The calculation result for Am(III) is shown in Table 6.5-2. It can be seen that even at such a high ligand concentration, the complexed americium is less than 2 percent of the total americium in the solution and is therefore negligible compared to free americium ions.

Table 6.5-2. Complexation of Am^{3+} with Intermediate Metabolites

Organic acid	Metal	Log K	Am Complexed
Formic	Am	1.2	0.08%
Acetic	Am	1.99	0.49%
Lactic	Am	2.43	1.33%

Source: NIST 2004 [DIRS 171201].

NOTE: Percentages of americium complexed are calculated by assuming the concentrations of intermediate metabolites to be 50 μM.

As mentioned above, another group of organic acids are microbial exudates, among which siderophores are of particular concern. Microbes require iron for DNA synthesis, electron transfer proteins, and nitrogen fixation. However, iron suffers from extreme insolubility in aerobic environments at physiological pH. Aerobic and facultatively anaerobic microorganisms have developed a system to acquire Fe(III). This is accomplished by siderophore generation. Siderophores are low molecular mass, ferric-specific ligands that are induced at low iron concentration for the purpose of biological assimilation of Fe(III). The most common siderophores contain the hydroxamic acid functional group -R-CO-N(OH)-R', which forms a five-membered chelate ring with Fe^{3+} (Hersman 1997 [DIRS 100763]). Because Fe(III) and Pu(IV) are similar in their charge/ionic radius ratio, Pu(IV) might serve as an analogue to Fe(III) (Hersman et al. 1993 [DIRS 100762]). However, in the repository, a large quantity of Fe(III) will be accumulated from oxic steel corrosion (Table 4.1-1), which will overwhelm Pu(IV) in complexation with siderophores. In addition, under oxidizing conditions anticipated in the repository, plutonium will be dominated by Pu(V) and Pu(VI), instead of Pu(IV) (Table 4.1-1). Therefore, the effect of siderophores for plutonium dissolution will be insignificant.

6.5.3 Biotransformation and Biosorption of Radionuclides

Microorganisms are known to accumulate radionuclides both extracellularly and intracellularly. In this section, possible processes of biotransformation and bioaccumulation of radionuclides by microorganisms are summarized based on open literature search. The relevance of these processes to the repository is then evaluated in the context of anticipated repository conditions.